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Estimated Optical Constants of Tagish Lake Meteorite

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Abstract

The visible, near-infrared, and mid-infrared (0.3-25 μm) real and imaginary indices of refraction are derived from reflectance measurements of the Tagish Lake meteorite. These are compared to some real and imaginary indices of refraction of the individual minerals composing the Tagish Lake meteorite. From this comparison it is clear that the imaginary indices of several individual minerals contribute to the estimated imaginary index of the Tagish Lake.

Introduction

The Tagish Lake meteorite (TLM) has been suggested as a spectral analog for D-type asteroids based upon comparisons of spectral color and slope (Hiroi et al. 2001). to the extent that this

correspondence of color (and albedo) is valid, then TLM can be considered a sample of one of the types of materials encountered in the outer solar system that may impart a characteristic red coloration to many of these surfaces (e.g. Wilson et al., 1994, Wilson and Sagan, 1995, Cruikshank et al. 1998a, Owen et al. 2001)

Theoretical modeling of the measured reflectance from planets and satellites has been used to infer information related to composition, grain size, and relative abundance of the surface components (Roush et al. 1990, Calvin and Clark 1991, 1993, Cruikshank et al. 1993, 1998a, Owen et al. 1993, 2001, Roush 1994, Wilson et al. 1994, Wilson and Sagan 1995, Grundy et al. 1999, Quirico et al. 1999, Douté et al. 1999, 2001, Buie and Grundy 2000). Such models inherently rely upon the optical constants, the real (n) and imaginary (k) indices of refraction, of candidate materials (see Roush et al. 1990, Roush 1994, and Cruikshank et al. 1998b, 1998c and references therein). If the optical constants of TLM were known, then these could be used for assessing whether or not this material can explain the range of color properties observed for outer solar system surfaces. In the following sections I discuss the derivation of the optical constants from a sample of TLM.

Analytical Approach

The approach combines two techniques. The first, originally described by Clark and Roush (1984), relies upon Hapke's formalisms that describe the reflectance from a particulate surface (Hapke 1981, 1986, 1993, and references therein) to derive k ; this technique has been applied to estimate optical constants of various materials (e.g. Calvin, 1990, Roush et al. 1990, Lucey 1998,

Cruikshank et al. 2001, and references therein). The second step uses a subtractive Kramers-Kronig analysis (K-K) to derive n from k (e.g. Warren 1984, and references therein).

The measured reflectance spectrum of TLM (sample grain diameter 125 μm , Hiroi et al. 2001) was used as a starting point in the analysis. Data from two different instruments were combined to cover the 0.3-25 μm region (Hiroi et al. 2001) and are shown in Figure 1a. The data at the longer wavelengths ($>1.6 \mu\text{m}$) exhibit a greater measurement variance, see the enlargement in Figure 1a, that will propagate into the derived optical constants.

In the first iteration, n is assumed invariant with wavelength (n_0). While this assumption may be reasonable for visible and near-infrared wavelengths, it becomes increasingly problematic at longer infrared wavelengths. At each wavelength an initial estimate of k is used to calculate the model reflectance and is then adjusted until the difference between the model and measured reflectance is 10^{-6} . The resulting k 's (k_1) are used in the K-K routine to determine n as a function of wavelength (n_1). In the second iteration, the n_1 's are used for the reflectance calculation and determination of k_2 's. The k_2 's are used in the K-K routine to determine n_2 as a function of wavelength. As shown in Figure 1b, the greatest difference ($\sim 8\%$) in n is occurs when n_0 is replaced by n_1 and little change is seen ($<0.5\%$) when n_1 is replaced by n_2 . Figure 1c shows that there is little difference ($<<0.2\%$) when k_2 replaces k_1 . This iterative refinement could continue indefinitely. However, the process is terminated after two iterations because the resulting n 's and k 's do not change significantly, as can be seen in Figures 1b and 1c.

Assumptions and Caveats

Several assumptions are made regarding most of the parameters associated with Hapke's equations, and a summary of these is provided in Table 1. The single scattering albedo (ω) is calculated from the n 's and k 's. The value of zero for both of the Legendre polynomial coefficients (b and c) corresponds to isotropic scattering. The value of unity for the relative amount of Fresnel reflectance from the front surface of the particles (β) implies euhedral grains. I assume a value of 0.05 (lunar-like surface) for Hapke's surface shadowing parameter (h). In principal h can be determined from microscopic characterization of the powdered sample of TLM or reflectance measurements over a broad range of viewing geometries, neither of which is available. Additionally, independent knowledge or assumptions about the grain size and n are required to determine n and k .

Assumptions regarding n are required for the reflectance calculations, as outlined above. The mineralogy of TLM has been described (Zolensky et al. 2002) but I am unaware of any reports that provide measurements of n . Table 2 summarizes the abundance and composition of the various components of TLM (Zolensky, pers. comm. 2001). Given these, n is estimated by weighting n 's of the individual minerals (n_i) (Deer et al. 1978, Egan and Hilgeman 1977) by their relative abundance (A_i), i.e. $\bar{n} = \sum n_i A_i$. Using this approach $\bar{n} = 1.6900$ (at $0.5893 \mu\text{m}$).

However, the reader is cautioned that using the relative mineral abundance and nominal densities to estimate the bulk density of TLM yields a value of $2.82^{+0.07}_{-0.09}$ g/cc which is significantly higher than the reported value of 1.66 ± 0.08 g/cc (Zolensky et al. 2002).

The grain size (diameter) used for the reflectance measurements was reported as 125 μm (Hiroi et al. 2001). For the initial analysis the median grain diameter was assumed (62.5 μm) and the associated k values are shown as the dotted line in Figure 1e. The sensitivity of the results to this assumption was investigated as follows. The maximum grain diameter (125 μm) was used in the calculation of the optical constants and the associated k values are shown as the solid line in Figure 1e. For the minimum grain diameter 15 μm was used in order to remain consistent with the inherent geometric optics assumptions of Hapke's theory to a wavelength of ~ 5 μm , the region dominated by reflected solar energy, and the resulting k values are shown as the dashed line in Figure 1e. In the strictest sense the results for the smallest assumed grain diameter are only valid at wavelengths ≤ 5 μm . Inspection of Figure 1e suggests that k 's derived exhibit an approximately inverse linear relationship as a function of assumed grain diameter. The means and associated standard deviations of the ratios $k_{62.5}/k_{125}$, k_{15}/k_{125} , and $k_{15}/k_{62.5}$, are 2.0 ± 0.00 , 8.34 ± 0.10 , and 4.17 ± 0.05 and correspond closely to the inverse ratio of grain diameters are 2.00, 8.33, and 4.17, respectively.

Comparisons to Mineral Optical Constants

There are published k 's for the various minerals identified in TLM (see Table 2). It is instructive to investigate if any of these individual minerals are contributing to the maxima seen in TLM k . Where possible, I compare to minerals whose composition is most consistent with those of TLM. However, TLM tends to be dominated by the Mg-rich silicates and k -values for these compositions are rare in the literature. Figure 2a shows the derived k 's for TLM and several

local maxima are labeled for purposes of the following comparison and discussion. The wavelength positions of these features are given in Table 3.

Values of k for serpentine and saponite are shown in Figure 2b. For serpentine the values of Mooney and Knacke (1985) are used, rather than those given by Roush et al. (1991), because they provide broader wavelength coverage and more importantly the sample has a Mg content more comparable to the serpentine in TLM (see Table 2). Values of k for two different optical axes of calcite and dolomite are shown in Figure 2c. Calcite data represent calculations for both optical axes based upon the oscillator parameters given in Long et al. (1993). Values of k for magnetite, olivine, and troilite are shown in Figure 2d. The original troilite data (Pollack et al. 1994) exhibit a discontinuity between 2 and 10 μm and is due to a lack of reported data between ~ 1 μm and 10 μm . More recent reports of the reflectance (Cloutis and Gaffey, 1994, Cloutis and Burbine 1999) and absorbance (Keller et al. 2002) of troilite do not directly support the presence of such a discrepancy. For the qualitative comparison below, the two disparate k data sets are simply scaled to the mean value between the longest wavelength of the Pollack et al. (1994) data and the shortest wavelength of the Begemann et al. (1994) data.

The wavelength positions of the maxima of the k values for these individual minerals are provided in Table 3. Inspection of Table 3 suggests that several minerals exhibit maxima close in wavelength position to those derived for TLM. For example, maximum in 1 TLM near 2.75 μm appears to have a sole candidate, serpentine, that has a similar feature near 2.72 μm . The feature is due to the metal-OH stretching fundamental of the structural hydroxyl located in serpentine. TLM feature 3 near 6.16 μm is well matched by the saponite is due to the bending

fundamental of molecular water. A variety of silicates can contribute to maxima 6, 7, and 9-11 due to the fundamental stretching ($\sim 10 \mu\text{m}$) and bending ($\sim 20 \mu\text{m}$) modes of the SiO_4 anion. For example, olivine has spectral features near TLM features 6, 7, and 11. Burns and Huggins (1972) identified seven spectral features that appeared in infrared transmission spectra of all olivine minerals in the forsterite-fayalite solid solution series. Every band showed a shift of the minimum position to higher frequencies (shorter wavelengths) with increasing Mg-content and might explain some of the discrepancies between the TLM and olivine positions given in Table 3.

Carbonates have three infrared active fundamental modes. Based upon a variety of measurements of calcite, White (1974) gives a range of $6.97\text{--}7.01 \mu\text{m}$ for the most intense band (ν_3), $11.35\text{--}11.47 \mu\text{m}$ for the intermediate strength band (ν_2), and $14.02\text{--}14.08 \mu\text{m}$ for the weakest band (ν_4) of calcite. Lane and Christensen (1997) give average values for calcite of $6.57 \mu\text{m}$ (ν_3), $11.32 \mu\text{m}$ (ν_2), and $14.04 \mu\text{m}$ (ν_4), but do not discuss the discrepancy for ν_3 . For dolomite, White (1974) gives positions of $6.97 \mu\text{m}$ (ν_3), $11.38 \mu\text{m}$ (ν_2), and $13.74 \mu\text{m}$ (ν_4), while Lane and Christensen (1997) cite average positions of $6.46 \mu\text{m}$ (ν_3), $11.19 \mu\text{m}$ (ν_2), and $13.74 \mu\text{m}$ (ν_4), again no discussion regarding the discrepancy of ν_3 is provided. Thus it appears that calcite and dolomite can contribute to a number of k features (4, 7, and perhaps 8) seen in the TLM data. The overtone and/or combination modes of these fundamentals give rise to spectral features at shorter wavelengths. In particular, carbonates exhibit spectral features near $4 \mu\text{m}$ (Hovis, 1966, Fink and Burk 1971, Blaney and McCord 1989, Salisbury et al. 1987, 1991, Wagner and Schade 1996) that are the most likely candidate for feature 2 seen in the TLM data.

The k of magnetite exhibits strong variation at the shortest wavelengths and a single broad feature near $17.5\ \mu\text{m}$. As a result, it may contribute to the TLM feature 9 that is rather broad and the strong slope in the TLM k at the shortest wavelengths.

The k of troilite exhibits strong variation at the shortest wavelengths and a broad feature near $23.5\ \mu\text{m}$. As a result, it may contribute to the TLM feature 10 that is rather broad and the strong slope in the TLM k at the shortest wavelengths.

Summary

Optical constants of Tagish Lake meteorite have been estimated from application of Hapke's theory (see Hapke, 1993, and references therein) and Kramers-Kronig analysis. These values are now available for modeling the reflectance spectra of objects in the outer solar system that exhibit a wide range of coloration. Although beyond the scope of the current investigation, it will be very interesting to assess whether or not the D-asteroid analog (Hiroi et al. 2001) of Tagish Lake can represent the coloring agent of the outer solar system objects through quantitative modeling.

A qualitative comparison of the estimated imaginary index of Tagish Lake to imaginary indices of individual minerals, identified in the meteorite from petrographic studies (Zolensky et al. 2002), illustrates how several individual minerals contribute to the signature of the meteorite.

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Table 1. Values of parameters used in derivation of the optical constants of Tagish Lake meteorite

Parameter	Use ¹	Value
ω	HRC	calculate from n and k
b	HRC	0.
c	HRC	0.
β	HRC	1.0
h	HRC	0.05
$n_{0.5893\mu\text{m}}$	K-K	1.6900

¹HRC is used in the Hapke reflectance calculation and K-K is used in the Kramers-Kronig calculation.

Table 2. Tagish Lake meteorite mineral abundance and composition

Mineral	Volume	Volume	Dominant	Reference	Reference
	Abundance	Abundance	Composition		mg
		(pore space corrected)			
Serpentine	26	29	Mg-rich (mg=0.99)	A	0.92
Saponite	26	29	mg~0.80	B	0.97
Carbonates	14	16	CaCO ₃	C	
			CaMgCO ₃	D	
			siderites		
Magnetite	12	13	Fe ₃ O ₄	E	
Troilite	5	6	(Fe,Ni) ₉ S ₈ , Fe _{1-x} S	F,G	
Olivine	6	7	Fe ₉₉	H	0.95
Pore Space	11	--			

mg=Mg/(Mg+Fe)

A. Mooney and Knacke (1985)

B. Roush et al. (1991)

C. Long et al. (1993)

D. Querry (1983)

E. Querry (1985)

F. Pollack et al. (1994)

G. Begemann et al. (1994)

H. Fabian et al. (2001), average of three optical axes

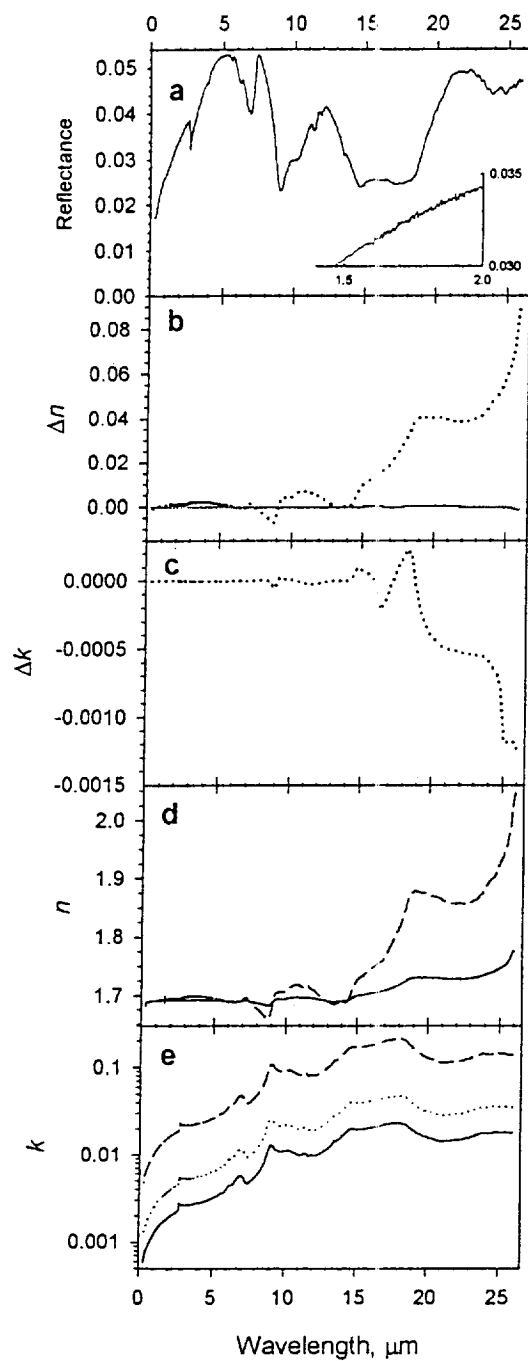
Table 3. Position of k maxima

Material	Maximum (μm)										
	1	2	3	4	5	6	7	8	9	10	11
TLM	2.74	3.98	6.16	6.95	9.05	10.24	11.42	13.52	14.64	18.15	24.75
Serpentine	2.72					10.5				16.1	22.7
Saponite			6.18			9.77			15.06		21.19
Calcite (ext)		Y					11.49				
Calcite (ord)		Y		7.09					14.00		
Dolomite (ext)			6.41				11.72	13.68			
Dolomite (ord)				7.01				13.70			
magnetite										17.7	
Olivine						10.25	11.41		16.54	19.05	24.97
						10.48	11.92			19.93	
Troilite							11.11		15.4		23.81

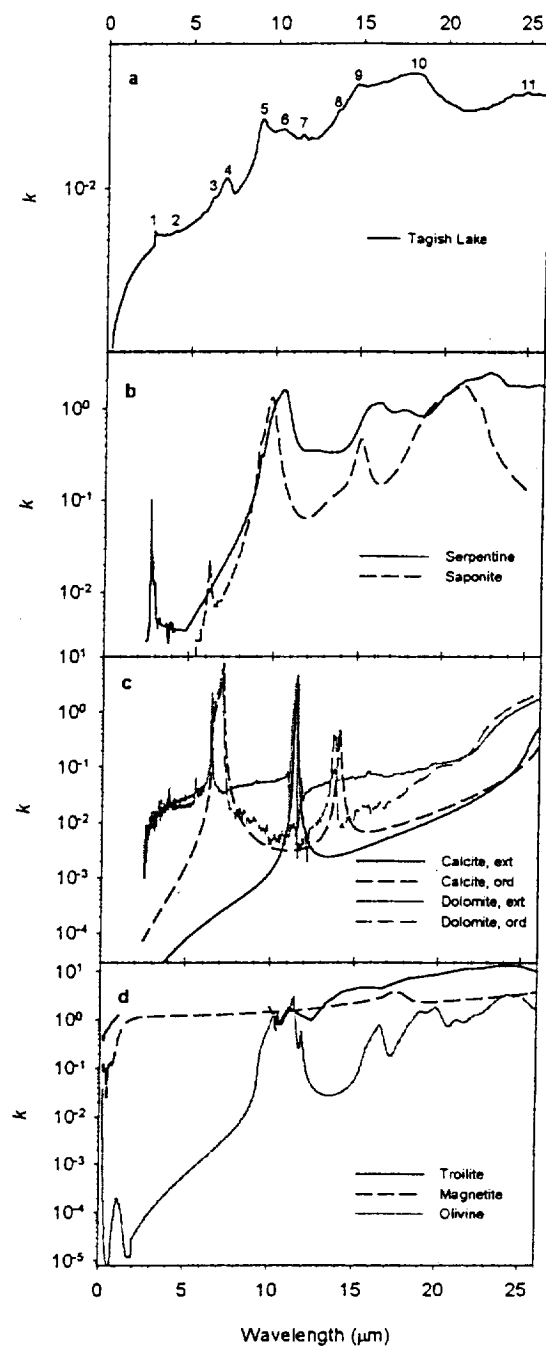
Figure Captions

Figure 1. (a) Measured reflectance of Tagish Lake meteorite from Hiroi et al. (2001). Inset enlarges the measurements from 1.4-3 μm where the peak-to-peak variability in the reflectance measurements is obvious. (b) Difference between n_0 and n_I (dotted line) and n_2 and n_I (light solid line). (c) Difference between k_2 and k_I . (d) Derived n for Tagish Lake meteorite assuming grain diameters of 125 μm (solid line), 62.5 μm (dotted line), and 15 μm (dashed line). (e) Derived k for Tagish Lake meteorite assuming grain diameters of 125 μm (solid line), 62.5 μm (dotted line), and 15 μm (dashed line).

Figure 2. Comparison of imaginary indices of refraction of various minerals to those derived for Tagish Lake meteorite. (a) Tagish Lake meteorite. Several maxima are labeled and their wavelength positions are given in Table 3. (b) Serpentine (black solid line) and saponite (black dashed line). (c) calcite extraordinary ray (black solid line), calcite ordinary ray (black dashed line), dolomite extraordinary ray (gray solid line), and dolomite ordinary ray (gray solid line) imaginary indices of refraction. (d) Troilite, (black solid line), magnetite (black dashed line), and olivine (gray solid line) imaginary indices of refraction. See text for sources of data and discussion.



Roush, Figure 1



Roush, Figure 2

